19. X—11   MICROCOMPUTERS IN CRYSTALLOGRAPHIC TEACHING.
By H. Schenk, Laboratory of Crystallography, University
of Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam,
The Netherlands.

Present-day microcomputers offer a wealth of computing
power at very limited costs. In fact, it is now well
possible, as we showed some years ago, to have a simple
least-squares structure refinement program running on
a $ 1000.- computer.

Another, and possibly more important, field in which
microcomputers can be applied is teaching. As a rule,
crystallographic methods depend heavily on computing,
and the associated programs are nearly always black
boxes which do not elucidate anything of what is going
on. To explain these methods to students, simulations
can be used. As an example, a direct method teaching
simulation on a microcomputer should leave all the
essential decisions to the students, and should itself
do only checking and administrative tasks, so that in
the end a student may grasp what's going on in the re-
search program. Other possibilities for computers in
teaching are of course computer-assisted instruction
and computer-managed instruction.

Along these lines, in the author's laboratory several
teaching programs have been developed, illustrating
Fourier Synthesis, Direct Methods, Model Building, etc.
and some results will be shown.

In the view of the author there should be set up an ex-
change for teaching programs which includes some referee
system. Only in this way programs already functioning in
a few laboratories will become available to the crystal-
lographic teachers at large.

Table 1

Pearson symbol	Structure type	Space group	Space group number
t I18	Al3Zr1	I4/mmm	139

Author
G.Brauer
1939 242 Pl   Monatsheft für Chemie
Remarks: also called Bi2SrlZnl,
Bi1 4(c), Bi2 4(e), Sr 4(e), Zn 4(d)

a = 0.4014   b = 0.4014   c = 1.732   [nm]
α = 90   β = 90   γ = 90   [degrees]
Origin at 4/mmm

Atoms	Site	Symmetry	X	Y	Z	occupancy
Al 1	4(c)	mmm	0.0	0.5	0.0	1.00
Al 2	4(d)	-4m2	0.0	0.5	0.25	1.00
Al 3	4(e)	4mm	0.0	0.0	0.361	1.00
Zr	4(e)	4mm	0.0	0.0	0.122	1.00

Followed by a table of compounds crystallizing in this structure type

Table 2

Phase	Space group	Structure type	a_b [nm] c	$α_β$ [D] $γ$	Atoms	point set	X	Y	Z	occ.
Hg2Na3	P42/mmm	Pearson	0.852	90	Hg	8(j)	.125	.125	.190	1.0
		symbol	0.852	90	Na1	4(c)	.0	.5	.0	1.0
		Hg2Na3	0.780	90	Na2	4(f)	.368	.368	.0	1.0
		tP20			Na3	4(g)	.210	.790	.0	1.0

Space lattice (c) (T) (p)	Remarks	Name Year	Coden Vol page
Structure like Al2Zr3 except Na1 in 4c not 4d; s.l. varies from 32 to 45 at% Hg, fig. given in ref. 2		Niels 1954	ACCRA9 7 277

19. 1—1   HANDBOOK OF CRYSTALLOGRAPHIC DATA FOR
INTERMETALLIC PHASES, P. VILLARS, L.D. Calvert and
W.B. Pearson, Eidgenössische Technische Hochschule,
Zürich, National Research Council of Canada and
University of Waterloo.

This handbook covers the world literature for this
area from 1913 to 1983. It includes all metallic
phases (elements, binary, ternary etc.) for which data
were found. Also included are simple oxides and
sulphides, but complex minerals and halogen containing
phases have been excluded.
This book is a critical evaluation of the best data
available and not a historical collection of structure
data. All type structures are given in standard
setting. The old data from the classical structure
compilations have been reevaluated and replaced where
necessary. For 1963-1983 the original literature
directly scanned covers over 20,000 publications, of
which around 15,000 contained useful citations. Part
1 is a handbook of all structure types (~1000)
ordered according to the Pearson symbol. A typical
entry is shown in Table 1.
Part 2 contains critically evaluated data for each of
the ~20,000 individual phases found. These are
alphabetically ordered and follow the pattern given in
Table 2.
This book is planned to be published in 1985.

19. 1—2   ATOMS, BONDS AND COMPUTERS. By I. D. Brown
and D. Altermatt, Institute for Materials Research,
McMaster University, Hamilton, Ontario, Canada L8S 4M1.

Computers are now widely used in organic and biological
chemistry for model building and data retrieval, but in-
organic chemistry is far behind because of the lack of a
simple ball and stick model to describe chemical struc-
ture and chemical connectivity.

The present project addresses two questions:

1. Can a computer, using only coordinates obtained
    from, for example, the Inorganic Crystal Structure
    Database, calculate a recognisable chemical
    description of the structure, i.e. can it identify
    the chemical bonds?

and

2. Can one use the resulting description of bonds for
    computer modelling of inorganic solids?

Considerable success has been achieved in answering the
first question with the program SINDBAD. This uses the
bond valence model that works well for compounds that
are formally ionic, i.e. contain bonds only between
anions and cations.

The program has 3 parts. In the first ranges are set
for interatomic distances that correspond to bonds. For
cation-anion bonds these are distances with bond valences
lying between 1.2 × (anion oxidation number) and 0.038 Å
(cation oxidation number). Anion-anion and cation-
cation bonds are only expected when both ions have less
than their maximum oxidation number. In the second part,
bond distances and bond valences are calculated and
checked to see if the bond valence sum around each atom
corresponds to its oxidation number. If it does not,
the third part of the program attempts to locate

possible errors in the input data. A systematic survey of structures in the Inorganic Crystal Structure Database shows that the program can provide a proper description of the chemical bonding for about 90% of the error-free entries and in 67% of these cases it can recognize that it has been successful. The output of this program is a listing of all the bonds formed by each cation and includes the bond length and valence, the bond vector and the symmetry transformation applied to the terminal atom (anion). This file is being used in the first instance to produce a bond index similar to that in BIDICS and later will be used to construct a connectivity index that can be searched by computer. Problems arise in constructing a connectivity index of inorganic solids from two sources – the continuous range of bond strengths present and the existence of networks with crystallographic translational symmetry. The former can be treated by allowing the user to define a threshold bond valence below which the bonding network is ignored. The latter requires careful treatment of the crystallographic symmetry by the computer so that the user can manipulate the structure without having to worry about space group operators and special positions.

These ideas can be extended to the predications of crystal structures. We have so far developed algorithms which successfully predict the chemical bonding network and bond lengths in most ternary compounds using only a knowledge of the coordination numbers and oxidation states of the constituent atoms. We hope to be able to solve the more complex problem of mapping the chemical bond network into the crystallographic bonding network once we have developed a proper description for the chemical connectivity in terms of the lattice symmetry.

19.1–4   STORING OF DATA OF OD-(ORDER-DISORDER) SUBSTANCES. By K.-O. Backhaus, H. Grell, Zentralinstitut für physikalische Chemie & H. Schrauber, Zentrum für Rechentechnik, Akademie der Wissenschaften der DDR, Berlin.

Besides the bibliographic file, OD specific data are stored. These are: The OD groupoid family with the net constants of the layers and parameters of the layer pairs. In detail are given: Atomic coordinates of atoms belonging to one OD layer, transformation matrices of the layer group and of the space transformations transforming one layer into the next layer. With this information deducing of any stacking of layers is possible, especially that of MDO structures or of periodic structures of any length. Simulated diffraction patterns allow comparison with the x-ray image of actually occurring substances.

Lit.: Backhaus, K.-O., Schrauber, H. & Grell, H.
CODATA 1983, Tagungsband, Seite 337.

19.1–3   CURRENT DEVELOPMENTS IN THE CAMBRIDGE STRUCTURAL DATABASE. By Olga Kennard, F.H.Allen, Sharon Bellard, J.E.Davies, J.Galloy, R.F.McMeeking, R.Taylor & D.G.Watson. Crystallographic Data Centre, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, England.

By 1st Feb. 1984 11,670 new entries had been added to CSD since the Ottawa Congress. The total database (41,725 entries) is now available in 25 countries. Additionally a number of major system developments are nearly complete :

Chemical Graphics. Programs have been developed to input, edit,store and display chemical structural diagrams. The current input is digitized via a Tektronix minicomputer; connectivity records are generated which contain 2D (x,y)-coordinates for each atom. Over 13,000 diagrams have now been input and published in Vols. 13-15 of MSD.To upgrade the backlog a program has been written to generate (x,y)-coordinates directly from the existing connection tables.

Integrated File Structure. The previously separate files of bibliographic, connectivity and numeric data have now been amalgamated into a single internal archive file. This complex undertaking required a major upgrade of CCDC internal software. Work is now directed towards a flexible structure for file releases to Affiliated Centres, suitable for a variety of computer installations.

New Search Strategies. The above integration means that bibliographic, connectivity and certain numeric items may now be searched together, rather than separately.To speed these searches a system of screens is being added to the file, based on numeric keys, hash-coding of text and bit screens for connectivity. Screenout rates of at least 96% have been achieved for a variety of bibliographic queries, leaving only 4% of entries for a full text match in the worst case. Ultimately the software will take advantage of chemical graphics to improve output. An enhanced system for query input is also planned.

19.2–1   COMPUTER ANIMATION AS AN AID TO CHEMICAL UNDERSTANDING

K M Crennell, G M Crisp
Computing Division
Rutherford Appleton Laboratory, SERC

L S Dent Glasser
Chemistry Department, University of Aberdeen

Computer Graphics is slowly displacing static mechanical models in popularity as an aid to the better understanding of chemical structure. We had no display devices working fast enough to show realistic moving structures and reactions, so we decided to use computer animation on film.

The III FR80 microfilm recorder was used to make a 16mm colour film, 'Silicates in Solution', which shows some of the possible mechanisms involved when silicates encounter water molecules in solution. Our approach to the problems of production is discussed, some typical computing times given and some still sequences from the film displayed.

Existing computer programs were used as far as possible; most of the moving sequences were made using PLUTO78, but we found it necessary to write a new one, TETRA, to simplify the manipulation of the shaded tetrahedra shown in the latter part of the film.